

MECHANISMS FOR SCALE DEPENDENCE OF THE EFFECTIVE MATRIX DIFFUSION COEFFICIENT

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RESEARCH OBJECTIVES

Matrix diffusion denotes the exchange of solute mass (through molecular diffusion) between fluid in fractures and fluid in the rock matrix. Owing to the orders-of-magnitude slower flow velocity in the matrix compared to that in fractures, matrix diffusion can significantly affect solute transport in fractured rock, and therefore is an important process for a variety of problems, including remediation of subsurface contamination and geological disposal of nuclear waste. The effective matrix diffusion coefficient is a key parameter for describing this matrix diffusion process. Our previous studies have indicated that the effective matrix diffusion coefficient values, obtained from a large number of field tracer tests, are enhanced in comparison with local values and increase with test scale. The major objective of this study is to investigate the physical mechanisms behind this scale dependence.

APPROACH

Numerical experiments were performed to evaluate the effects of flow-path geometry in a fracture network (Liu et al., 2007a). The focus of the experiments was on solute transport in flow paths having geometries consistent with percolation theories and characterized by local flow loops formed mainly by small-scale fractures. Values for effective transport parameters were obtained by matching breakthrough curves from numerical experiments with an analytical solution for solute transport along a single fracture. To investigate the effects of property heterogeneity on the rock matrix, we also derived analytical expressions for the effective matrix-diffusion coefficient for two idealized fracture-matrix systems: a single fracture system associated with rock matrix heterogeneity along the water flow direction in the fracture, and a multiple fracture system with rock-matrix heterogeneity among different fractures (Liu et al., 2007b). These analytical results allow for direct demonstrations of relationships between the scale dependence and spatial variability of the rock-matrix diffusive properties.

ACCOMPLISHMENTS

Our study indicates that the observed scale-dependence of the effective matrix diffusion coefficient results from a combination of flow-path-geometry effects and the heterogeneity of rock-matrix diffusive properties. Numerical experiment results show that the matrix diffusion process associated with local

flow loops formed by small-scale (or high-level) fractures (which is mostly ignored in current modeling practices) seems to be an important mechanism in causing the observed scale dependence (Figure 1). Our analytical results further demonstrate that different-scale heterogeneities of the rock-matrix diffusive properties also contribute to this scale dependence.

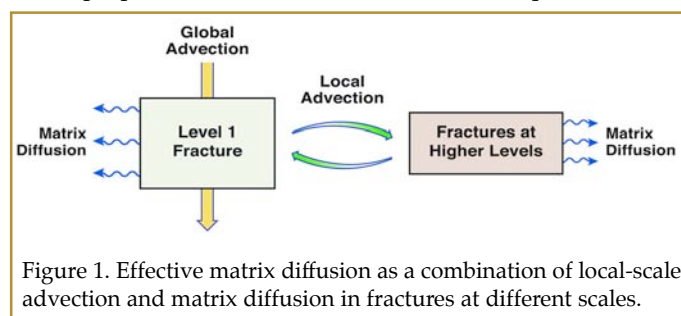


Figure 1. Effective matrix diffusion as a combination of local-scale advection and matrix diffusion in fractures at different scales.

SIGNIFICANCE OF FINDINGS

While the scale dependence of permeability and dispersivity has been an active research topic for many years, this study shows that the effective matrix diffusion coefficient, an important parameter controlling matrix diffusion processes, is also scale dependent. This finding has many important implications for problems involving matrix diffusion, including remediation of subsurface contamination in fractured rock and geological disposal of nuclear waste.

RELATED PUBLICATIONS

- Liu, H.H., Y.Q. Zhang, Q. Zhou, and F. J. Molz, An interpretation of the potential scale dependence of the effective matrix diffusion coefficient. LBNL-60744. *Journal of Contaminant Hydrology*, 90(1-2), 41-57, 2007a.
- Liu, H.H., Y. Zhang and F. J. Molz, Scale dependence of effective matrix diffusion coefficient: Some analytical results. LBNL-60746. *Vadose Zone Journal* (in press), 2007b.

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